STUDY PACK : 2

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The Core Principles of Chemistry

ATOMIC STRUCTURE & THE PERIODIC TABLE

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Atomic Structure

1. Define the following,

(a) Elements :

Substances which cannot be split into simpler substances. Elements are composed of atoms of the same kind.

(b) Compounds:

Pure substances which can be split into simpler substances. Compounds are formed by the combination of two or more atoms chemically bonded.

(c) Atom :

Atom is the smallest, electrically neutral particle of an element or compound which cannot exist on its own & they do take part in chemical reactions.

(d) Molecule :

A molecule is the smallest electrically neutral particle of an element or compound which can exist on its own, and is formed by the union of atoms chemically bonded.
Eg: H_2, O_2, Cl_2

(e) Ion :

An ion is an atom or group of atoms, which carries an electric charge.

2. Describe the simple model of an atom

The atom is mostly empty space. It has a solid core known as nucleus in the center, which consists of protons and neutrons. The electrons circulate around the nucleus in specific orbitals or shells.

3. What are sub atomic particles? Describe each of them

Protons – Has a unit positive charge and a mass of 1 RAM, found in the nucleus.

Neutrons – Has a mass of 1 RAM and no charge found in the nucleus.

Electrons – Negligible mass, negatively charged, rotates around the nucleus.

4. State the masses & electric charges of sub atomic particles

Particle	Relative mass	Relative Charge

5. Describe the behavior of beams of protons, neutrons & electrons in electric fields

6. Define the terms "**Mass number**" & "**Atomic number**" of an atom & state their Inter relationship

Mass number (<u>nucleon number</u>) : The total of protons & neutrons of an atom

Atomic number (<u>proton number</u>) : Number of protons of an atom

The mass number is roughly double the atomic number

7. How do you calculate the number of neutrons in a given atom?

No. of neutrons = Mass number- atomic number

8. What is the relationship between the no. of protons & the no. of electrons of an atom?

They are equal

9. What are Isotopes? Name some examples for isotopes

Isotopes are different atomic forms of the same element which has the same atomic number but different mass number.

(Definition in terms of sub atomic particles) Isotopes are different atomic forms of the same element which has the same number of protons but different number of neutrons.

Eg:

10. What you can comment on the chemical behavior of isotopes? Are they same or different? Explain your answer

The chemical behavior depends on the no. of electrons. The isotopes contain the same no. of electrons, but different no. of neutrons. Therefore the isotopes exhibit similar chemical properties.

11. Explain why the relative atomic mass of chlorine is 35.5 and not a whole number?

Chlorine exist as two isotopes ^{35}Cl & ^{37}Cl each 75% & 25% respectively. Below relative atomic mass calculation proves the R.A.M of Chlorine is 35.5 & not a whole number.

R.A.M = 35 x 75/100 + 25 x 25/100

35.5

12. How many electrons, neutrons and protons are present in the following nuclides?

${}^{1}_{1}H$ ${}^{16}_{8}O$ ${}^{14}_{6}C$ ${}^{23}_{11}Na$ ${}^{31}_{15}P$ ${}^{35.5}_{17}Cl$ ${}^{32.1}_{16}S$

e :

p :

n :

${}^{24.3}_{12}Mg^{2+}$ ${}^{27}_{13}Al^{3+}$ ${}^{14}_{7}N^{3-}$ ${}^{79.9}_{35}Br^{-}$ ${}^{28.1}_{14}Si^{4+}$

e :

p :
n :

Atomic Mass

1. Explain why the mass of an atom is measured in relative masses?

The mass of an individual atom is very small therefore it is only possible to measure the atomic masses in relative masses. Since SI units cannot be used, we use an atom itself to measure the mass of another atom

2. Define "**Relative atomic mass**" ? Write its units.

$$\text{R.A.M} = \frac{\text{The average mass of an atom of an element}}{\text{1/12}^{\text{th}} \text{ the mass of an atom of } {}^{12}_{6}\text{C isotope}}$$

No units

3. Define "**Relative molecular mass**"? Write its units.

The sum of the relative atomic masses of a molecule is the relative molecular mass.
No units.

4. Define "**molar mass**"? Write its units.
Molar mass is the mass of one mole of the of a substance
Unit : g mol^{-1}

5. Calculate the Relative molecular mass & molar mass of these molecules

$(NH_4)_2SO_4$

$Pb(NO_3)_2$

$Ca(HCO_3)_2$

$(COOH)_2.2H_2O$

$Na_2SO_3.5H_2O$

$CuSO_4.5H_2O$

$Cu(NH_3)_4SO_4.2H_2O$

6. Define "**Relative isotopic mass**"?

$$R.I.M = \frac{\text{The mass of an atom of an isotope}}{1/12^{th} \text{ the mass of an atom of } {}^{12}_{6}C \text{ isotope}}$$

No units.

7. i) The relative abundance of "Cl" isotopes are ^{35}Cl - 75% & ^{37}Cl - 25%. Calculate the relative atomic mass (RAM)of "Cl"?

ii) Two isotopes of "X" exists in nature as ^{16}X & ^{18}X, the relative abundance of ^{16}X is 70%, find the relative atomic mass of "X"?

Mass Spectrometer

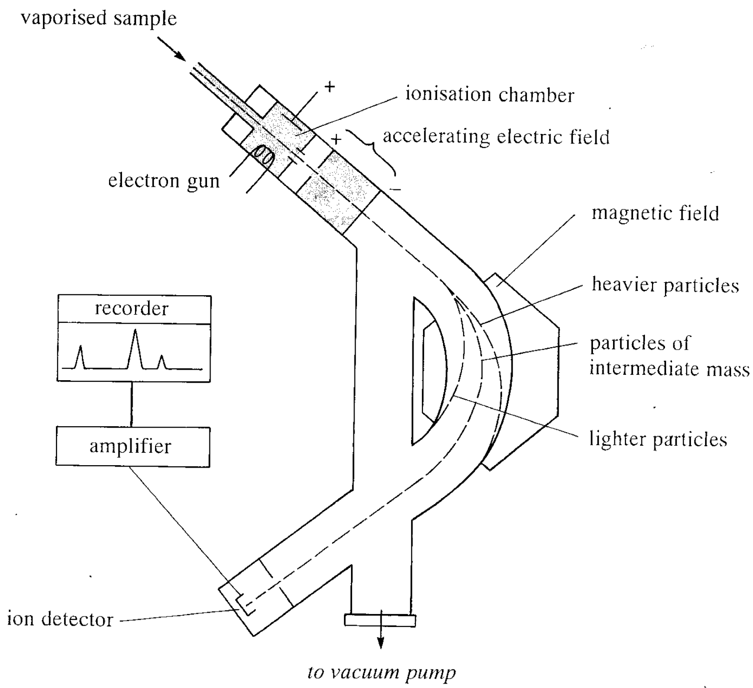
1. What is mass spectrometer?

The mass spectrometer is an instrument used for accurately measuring atomic masses & for finding the number of isotopes of an element by separating the positively charged gaseous particles as to their mass/charge ratio.

2. Name the main five sections of a mass spectrometer

1. Vaporizer - The sample is vaporized
2. Ionizer - Positive ions are obtained
3. Accelerator - Positive ions are accelerated by an electric field.
4. Deflector - Positive ions are deflected by a magnetic field.
5. Detector - Ions are detected & a record is made.

3. Detailed labeled diagram of a mass spectrometer



4. Describe briefly how a mass spectrometer works stating the principle of each stage

The mass spectrometer separates positively charged gaseous particles according to their mass/charge ratio thus detect their presence by an ion detector.

i. Vaporization:-

The sample is introduced into the vaporizing chamber; before it passes onto the ionizing chamber the sample is completely vaporized. The particles present in gaseous state can be gaseous atoms, compounds or molecules.

ii. Ionization:-

After vaporization, the molecule passes in to the ionization chamber, where atoms of the element are bombarded by a stream of high energy electrons. This causes ionization resulting positively charged ions. One or two electrons are knocked out of the atoms leaving cations. Mostly uni positive cations are produced sometimes dipositive ions may also be produced.

$$A_{(g)} + e \longrightarrow A^{+}_{(g)} + 2e$$

iii. **Acceleration:-**

These cations pass through the electric field. Thus ions are accelerated by the electric field.

iv. **Deflection:-**

The magnetic field deflects the particles according to their mass/charge ratio. The particle with the highest mass / charge ratio will deflect less due to its greater kinetic energy & the particle with the least mass/charge ratio will deflect more.

v. **Detection:-**

When a positively charged particle reaches the ion detector, it will produce a signal thus will be amplified to a computer and a record will be made.

5. Describe some **modern uses** of mass spectrometers

- **Radioactive dating :**

The relative amounts of ^{12}C & ^{14}C in a sample can be found by mass spectrometer. ^{14}C is radioactive and it has a half-life of 5730 years as it changes to N.
The difference between the historical ratio & the measured amount in the mass spectrum of a carbon containing substance is the basis of carbon dating.

- **Space research:**

Identification of elements present in a sample of rock from various planets. The rock sample is subjected to a mass spectrometer inorder to identify the composition of the sample.

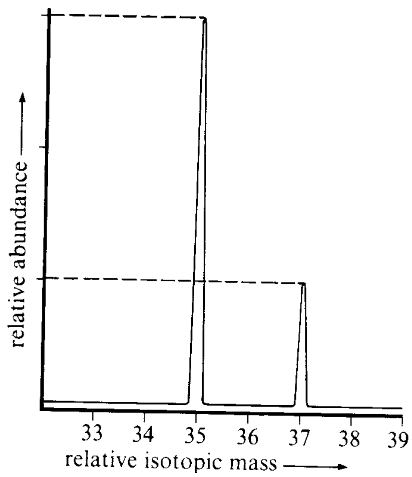
- **In sport to detect use of anabolic steroids:**

Urine sample from athlete is taken & placed in a mass spectrometer. If the athlete has consumed steroids such as nandrolone there will be a peak m/e equivalent to that of the molecular ion of nandrolone.

- **In the pharmaceutical industry to provide an identifier for compounds synthesized for possible identification as drugs:**

The identification identity of a new compound or to find out the presence of a certain chemical is done by measuring the m/e value of the peak caused by the molecular ion. The use of laser energy instead of temperature in the mass spectrometer is done inorder to prevent the decomposition of fragile molecules.

6. The Mass Spectrum trace for Chlorine is shown below

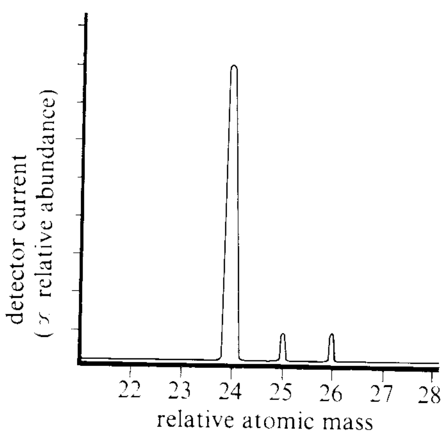


Calculate the;

I. Relative abundance of each isotope ^{37}Cl & ^{35}Cl

II. Relative atomic mass of Chlorine

5. The Mass Spectrum trace for Magnesium is shown below



Calculate the;

I. Relative abundance of each isotope of 'Mg'

II. Relative atomic mass of Magnesium

6. If a mono atomic element is introduced into the mass spectrometer

   a. How many different particles will you expect in the ionizing chamber?

   b. What are the factors, which is responsible for the number of particles to differ from one mono atomic element to another?

c. Rubidium has two isotopes ^{85}Rb & ^{87}Rb and if the ionizing chamber forms both +1 &+2 ions, write the formulae & the m/e values of all the species you would expect to find in the ionizing chamber

d. Relative abundances of the isotopes of Rubidium are ^{85}Rb 72.12% & ^{87}Rb 27.88%, Sketch a mass spectrum you would expect from a sample of 'Rb' & calculate the Relative Atomic Mass.

7. Interpret the mass spectrum by making the terms molecular ion, fragmentation, & base peak clear.

A mass spectrum is presented as a bar graph. Each peak in the spectrum represents a fragment of the molecular ion. Molecular ion is an ion formed by a molecule by the loss of one electron.

Eg: $Cl_2 - e \longrightarrow Cl_2^+$

When the molecule is passed into the ionization chamber, an electron is knocked off to give a molecular ion M^+ (sometimes referred to as the parent ion), or sometimes given the symbol M^+.

$$\underset{\text{(high energy)}}{M + e^-} \longrightarrow \underset{\text{(molecular ion)}}{M^+ + 2e^-}$$

❖ In the mass spectrum the ion with the greatest m/e value is the molecular ion.

These molecular ions are energetically unstable, hence some will fall apart to result in an atomic ion and the atom itself (Radical). The breakdown of the molecular ion in this manner is referred to as fragmentation.

$$Cl_2^+ \longrightarrow Cl^\cdot + Cl^+$$

The atom is not ionized in the ionization chamber, nor accelerated or deflected, will it be removed by the vacuum.

❖ The patterns of lines, of a mass spectrum of an **element** is related to the number of isotopes. Each line represents a different isotope of that element. With a compound, each line represents a different fragment produced when the molecular ion breaks up.

❖ The relative sizes of the peaks is a direct measurement of the relative abundances of isotopes or fragments. The relative abundances are found by measuring the lines on the stick diagram.

❖ The tallest (most intense) peak in a spectrum is called the base peak. The base peak represents the common most fragment ion formed and is usually given an arbitrary value of 100 (relative intensity of 100) and the height of other peaks are measured relative to this.

10. Sketch the mass spectrum of a chlorine molecule & explain how various fragmentations & peaks occur.

As chlorine consists of molecules, not individual atoms, it produces Cl_2+ molecular ion at the ionization chamber. Some of these unstable molecules undergo fragmentation as shown below & some remain as Cl_2+

$$Cl_2^+ \longrightarrow Cl^{\cdot} + Cl^+$$

As 'Cl' has two isotopes Cl^{35} & Cl^{37} in the approximate ratio of 3 atoms of Cl^{35} to 1 atom of Cl^{37}. It will produce lines at m/e 35 & 37. There are 3 possible combinations for the Cl_2^+ ion

Energy levels, Orbitals & Shells

1. Explain how electrons are occupied in energy levels

Electrons are distributed in energy levels and they fill up such that each electron occupies the lowest possible energy levels.

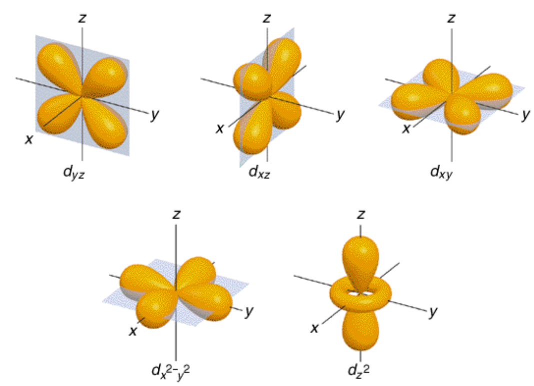
a. First energy level has 1 sub-level. **(s-orbital)**

b. Second energy level has 2 sub-levels. **(s and p orbital)**
c. Third energy level has 3 sub-levels. **(s, p and d orbital)**
d. Fourth energy level has 4 sub-levels. **(s, p, d and f orbital)**

2. Describe the s and p sub Orbitals & sketch their shapes

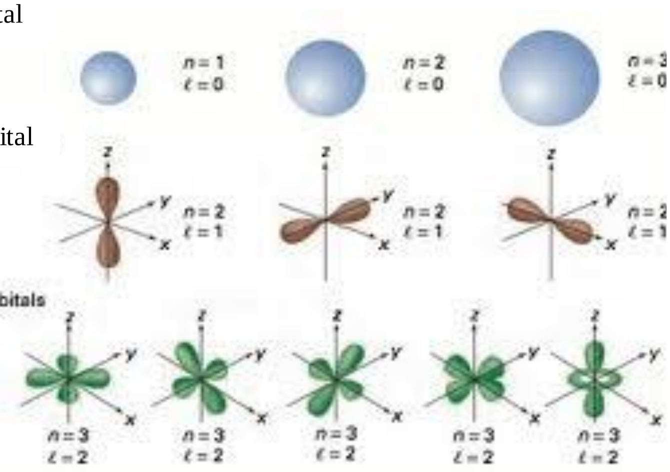
The sublevels are defined according to the shape in which the electrons can orbit.

d-orbital



s-orbital

p-orbital



Each it. Each orbit can occupy 2 electrons but they are of opposite spin.

3. Explain the below terms :

a) Aufbau approach:-

The building up principle according to each electron occupying the lowest possible energy level is called the Aufbau approach.

b) Pauli Exclusion Principle :-

The 2 electrons in an atomic orbital has different spin (electrons orbit in opposite spin) is called the pauli exclusion principle.

c) Hund's Rule :-

Any p,d or f sub level the building up is such that the orbitals in the sublevel are first singly occupied by electrons before they are doubly occupied.

4. Write the **electronic configuration** of elements from <u>Hydrogen</u> to <u>Krypton</u> using the building-up principle (using 1s,2p… notation & electron-in-boxes notations)

^{1}H : $1s^1$

[|]

^{2}He : $1s^2$

[||]

^{3}Li : $1s^2$ $2s^1$

[||] [|]

^{4}Be :

^{5}B :

^{6}C :

^{7}N :

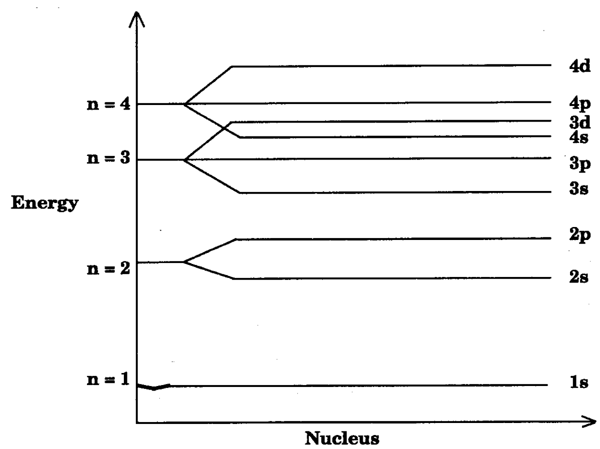
^{8}O :

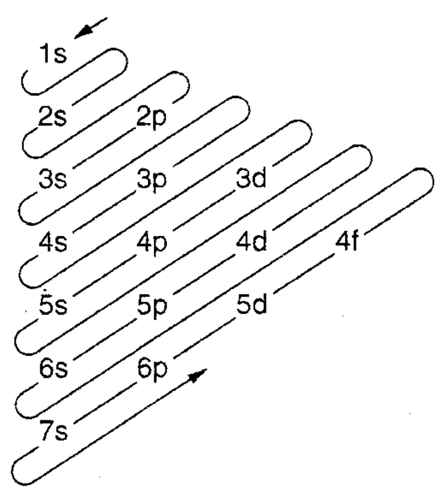
^{9}F :

^{10}Ne :

^{11}Na :

^{12}Mg :





^{13}Al :

^{14}Si :

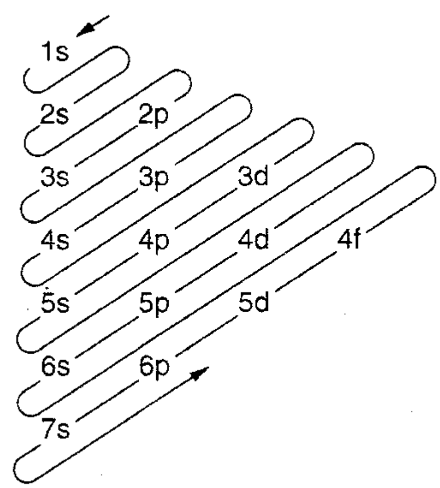
^{15}P :

^{16}S :

^{17}Cl :

^{18}Ar :

^{19}K :



^{20}Ca :

^{21}Sc :

^{22}Ti :

^{23}V :

^{24}Cr* :

^{25}Mn :

^{26}Fe :

^{27}Co :

^{28}Ni :

^{29}Cu* :

^{30}Zn :

^{31}Ga :

^{32}Ge :

^{33}As :

^{34}Se :

^{35}Br :

^{36}Kr :

5. Write the **electronic configuration** below ions using the building-up principle (using 1s,2p… notation & electron-in-boxes notations)

$^{7}N^{3-}$:

$^{8}O^{2-}$:

$^{11}Na^{+}$:

$^{12}Mg^{+}$:

$^{13}Al^{2+}$:

$^{15}P^{3-}$:

$^{17}Cl^{-}$:

$^{25}Mn^{2+}$:

$^{26}Fe^{2+}$:

$^{26}Fe^{3+}$:

$^{29}Cu^{2+}$:

$^{30}Zn^{+}$:

6. Describe how electronic structures determines the chemical properties of an element

Chemical reactivity depends on the number of electrons in the outermost energy level and therefore one could predict that elements with the same number of electrons in the outer energy level would have similar chemical properties. All elements with the same number fall into the same group.

7. Define the following terms: -

a. First electron affinity:-

The energy released when 1 mole of gaseous atoms gains one mole of electrons to form a mole of uni-negative gaseous ions, always exothermic.

$X_{(g)} + e \longrightarrow X^{-}_{(g)} \quad \Delta H(\text{-ve})$

b. Second electron affinity:-

The energy absorbed when 1 mole of uni negative gaseous ions gains 1 mole of electrons to form 1 mole of di negative anions, always endothermic.

$X^{-}_{(g)} + e \longrightarrow X^{-2}_{(g)} \quad \Delta H(\text{+ve})$

7. Explain why the second electron affinity is always endothermic

Repulsion from the electron of the negative ion and the incoming electron makes it necessary for the incoming electron to have enough energy to overcome the repulsion. Therefore the 2nd electron affinity is endothermic.

Ionization Energy

1. What is ionization energy?

The energy, which is needed to remove any electron away from gaseous atoms. As the nucleus attracts the electrons, the removal of it requires energy in order to overcome the attractive force. Therefore the energy of ionization is endothermic.

2. Define the following terms

a) First ionization energy :-

The first ionization energy is the heat energy required to remove 1 mole of electrons from a mole of gaseous atoms to form a mole of uni positive gaseous ions.

$M_{(g)} - e \longrightarrow M^{+}_{(g)}$ Δ H(+ve)

b) Second ionization energy :-

The heat energy required removing 1 mole of electrons from a mole of uni positive gaseous ion to form a mole of di positive gaseous ions.

$M^{+}_{(g)} - e \longrightarrow M^{+2}_{(g)}$ Δ H(+ve)

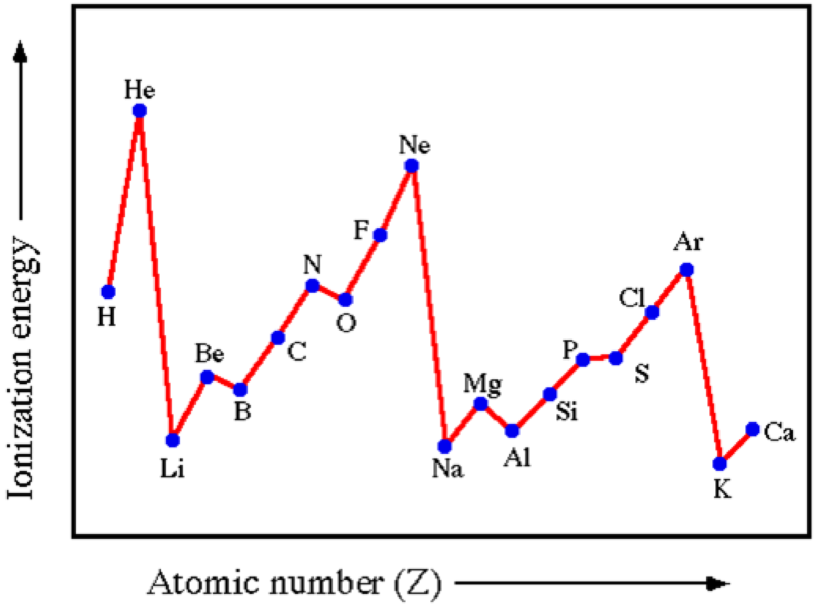
c) Third ionization energy:-

The heat energy required removing 1 mole of electrons from a mole of di positive gaseous ion to form a mole of tri positive gaseous ions.

$M^{2+}_{(g)} - e \longrightarrow M^{+3}_{(g)}$ Δ H(+ve)

3. **State the factors influencing the ionization energies of elements**

4**. Plot the first Ionization energy of the elements 'H' to 'Ar' against their atomic numbers**



5. Explain the variation of 1st ionization energy down a group & across a period.

- The size of the atom decreases across a period due to increased nuclear attraction, which is result of increased atomic number. Therefore the effective nuclear attraction generally increases across a period resulting an increase in the first ionization energy.
- The first ionization energy decreases down a group due to electrons being less attracted by the nucleus due to the following 2 reasons.

a) As the number of shells increases, the distance between the nucleus and the outermost electron increases resulting less nuclear attraction.

b) As the number of shells increases, the shielding numbers of electrons also increase causing the effective nuclear charge to decrease (effective nuclear charge is the charge felt on each electron). Therefore, the first ionization energy decrees down the group.

6. Explain what is shielding/ screening effect?

- The inner electrons causes the nuclear charge felt on the outer electrons to reduce. Thus the effect of the inner electrons in reducing the charge experiend by the outer electrons is called shielding/screening effect.
- As the number of shells increases, the shielding or screening effect will increase.

7. Explain the drop in the ionization energy between Be-B & N-O in the 2nd period, also between Mg-Al & P-S in the 3rd period

Electronic configuration for 'Be' & 'B' shows that 'B'e has a stable S^2 configuration than that of 'B'.

$^{4}Be = 1s^2, 2s^2$ $^{5}B = 1s^2, 2s^2\ 2p^1$

To remove an electron from 'Be' requires more energy due to its stability. Fully filled or half-filled orbital (e.g.: S^2,P^3,P^6,d^5,d^{10}) are more stable. Therefore they show unexpected high first ionization energy.

Also the electronic configurations for N & O will explain why N has high ionization energy.

$^{7}N = 1s^2, 2s^2 2p^3$ $^{8}O = 1s^2, 2s^2\ 2p^4$

The outer electrons in 'N' are in p3 stable form. Therefore needs lot of energy to remove an electron from 'N' .unlike in 'O' where the paired electron in the p-orbital results in repulsion between them. This makes it easier, for the electron to be removed. But the second ionization energy of oxygen will be greater due to the stable p3 configuration.

The variation of the first ionization energy of Mg to Al and P to S can be explained in a similar manner.

Mg Al

P S

8. State the relationship between the atomic number & the successive ionization energy

A single atom of an element will have number of successive ionization energies.(successive ionizations involves removal of all the electrons of the atom) The total of all possible successive ionization energies will be equal to the total number of electrons, which therefore in an atom will be equal to the atomic number.

9. Explain the variation of successive ionization energy as the ionization of the atom increases.

• The ionization energy depends on the attraction of the electrons to the nucleus. For the first ionization energy, the nuclear attraction per electron will be less than after the second ionization where the effective nuclear attraction increases as electrons are removed.

• Therefore, each successive ionization energy will be greater than the one just before it. This means the successive ionization energy increases as the number of ionization increase.

10. Explain how the successive ionization energies provide evidence for the existence of quantum shells (energy levels)

• The irregular increase in the ionization energy will show how many energy levels (quantum shells) the element will possess.

• There will be a large increase in the ionization energy when the electrons are removed from a new energy level. Therefore by observing the huge difference we can conclude the number of quantum shells, thus period number.

Eg:-

I. What are the information, which we can gather from successive ionization energies of an element?

1. <u>Atomic number:</u>
   The total number of successive ionization equals the atomic number.

2. <u>No. of quantum shells:</u>
   The number of changes with significant large increase gives the number of energy levels.

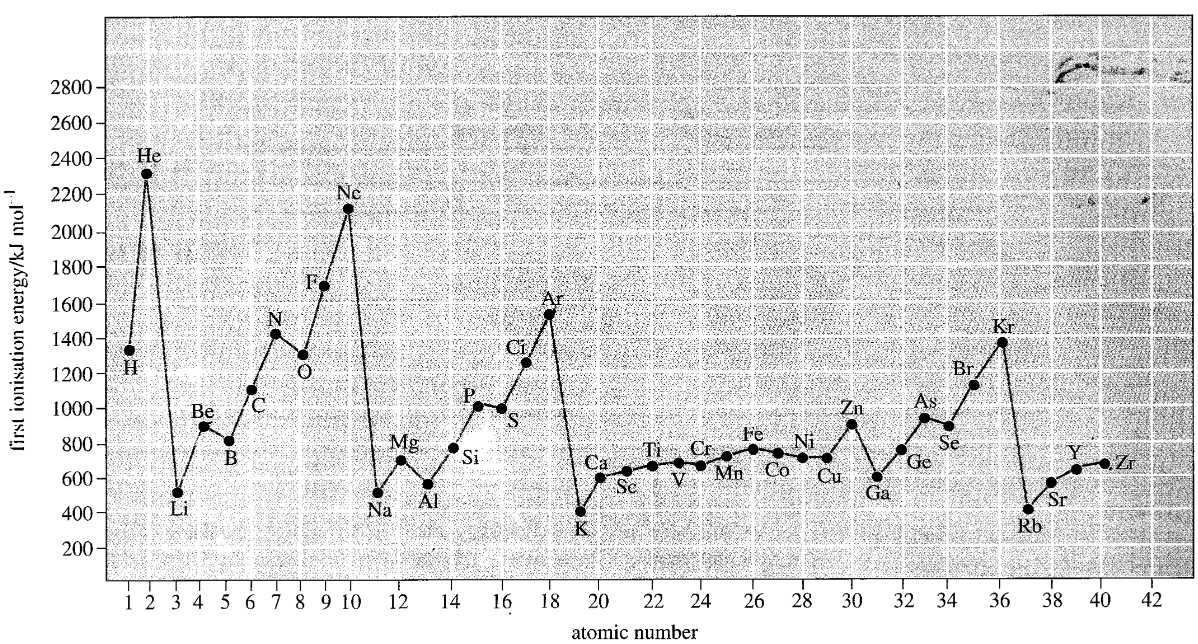
E.g.: One Significant large change means there are 2 energy levels.
Two significant large changes means 3 energy levels.

3. <u>Group Number :</u>

The number of successive ionization before the first significant large change gives the number of electrons in the highest energy level (outermost shells). Therefore the group number can be predicted.

II. Plot a sketch of successive ionization energies for Sodium.

11. Explain how 1st ionization energies of successive elements provide evidence for the existence of characteristic energy levels of s, p, d-Orbitals, using below graph



The graph between 1 noble gas and the next can be divided into subsections. These subsections contain either 2,6 or 10 points on the graph.

E.g.: Li to Be and Na to Mg → 2 points
B to Ne and Al to Ar → 6 points
Sc to Zn → 10 points.

These subsections of points correspond to sub shells of electrons. By studying the energy of ionization we can conclude that:

n=1 (first shell) contains 2 electrons in the same sub shell (s-orbital)

n=2 shell contains 2 electron in 1 sub level (s-orbital) and 6 electron in slightly higher level (p-orbital)

n=3 shell contains 2 electron in 1 sub level (s-orbital),6 electrons in slightly higher sub level (p-orbital)and 10 electrons in to still slightly higher sublevel (d-orbital)

PERIODIC TRENDS

1. Define the term 'periodic property'

A periodic property is a characteristic of atoms that varies regularly across the periodic table.

2. Explain the factors to be considered when determining boiling and melting points of elements across the periods.

For simple Covalent molecules the boiling and melting point depends on the strength of the Vander Waal's forces between the molecules, not the strength of the covalent bond within the molecule, except in giant atomic solids (often referred to as giant molecular) or ionic compounds. When a giant atomic (giant molecular) solid such as diamond or graphite is heated, the covalent bonds between the atoms are broken. But the covalent bonds are not broken when a simple molecular substance is boiled or melted. Therefore the strength of the covalent bonds within the molecules does not influence the boiling and melting points of a molecular substance.

The melting & boiling points tell us how strongly the ions in an ionic compound held together. If it a metal how strong the metallic bond is. If the compound is a simple covalent then the strength of the Vander Waals attraction determines the melting & boiling points if it is ionic then the strength of the ionic bond determines the melting and boiling point. For metals the strength of metallic bond determines the boiling and melting points.

3. Explain the trends in melting and boiling temperatures of elements of period 2 & 3 in terms of structure and bonding.

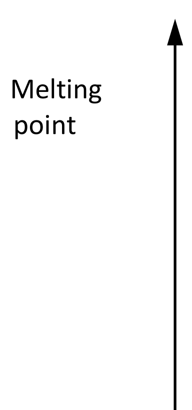
From 'Li' to 'B' the strength of the metallic bond increases due to increased number of delocalized electrons & decrease ionic radii. As a result the melting point increases from Li-Boron.
Carbon will exhibit the highest sublimation point. Melting Carbon involves braking of all four covalent bonds around each carbon atom in the giant atomic solid.

Elements from 'N' to 'Ne' form simple covalent molecules such as N_2, O_2, Cl_2 the melting point decreases due to decrease in the strength of dispersion forces (a type of Vander Waals force) Strength of dispersion force depends on number of electrons. As the number of electrons decrease the boiling & melting points decrease from N-Ne.

From 'Na' to 'Al' the strength of the metallic bond increases due to increased number of delocalized electrons & decrease ionic radii. As a result the melting point increases from Na-Al.

'Si' forms giant atomic structures (giant molecular) similar to diamond where the melting point is extremely higher. Melting 'Si' involves breaking of all four covalent bonds.
Elements from 'P' to 'Ar' form simple covalent molecules such as P_4, S_8 the melting point decreases due to decrease in the strength of dispersion forces which depends on number of electrons.

4. Plot a graph to show the variations of melting points against the atomic number of period 3 elements



Atomic number